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NOLTR 62-84

A MAGNETIC TAPE LIBRARY OF THERMODYNAMIC DATA

15 MAY 1962

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Page 11. After reference 18, add the following:

19. J. S. Martinez and G. W. Elverum, Jr., A Method of Calculating the Performance of Liquid Propellant Systems. Jet Propulsion Laboratory, Report 20-21 (Dec., 1955).

20. L. Brewer and A. W. Searcy, The Gaseous Species of the Al-Al_2O_3 System. J. Am. Chem. Soc. 73, 5308 (Nov., 1951).

21. Janaf Thermochemical Data - 2 Vols., Dow Chemical Company (Dec., 1960) and Supplements.

22. Proceedings of the First Meeting, Janaf Thermochemical Panel, Publication No. T-1 (Nov., 1959).

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NOLTR 62-84

A MAGNETIC TAPE LIBRARY OF THERMODYNAMIC DATA

Prepared by:

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ABSTRACT: This report describes the production and use of a magnetic tape library of thermodynamic data. The tape is produced from a deck of punched cards, six for each of more than one hundred chemical species. The data on each species include an identification number, coded references, formula, and atomic weight (of elemental species), the enthalpy change from 0°K to 298.15°K, the standard heat of formation at 298.15°K, melting point and heat of fusion, boiling point and heat of vaporization, coefficients giving the specific heat as a rational function of the temperature, and integration constants permitting calculation of enthalpy and entropy. All data are given for a pressure of one atmosphere. These data permit calculation of enthalpy, entropy and the Gibbs free energy over the temperature range 1000° - 6000°K. The machine program used in the work is presented accompanied by illustrations of its use. Sources of the original data are given. Examples are produced from the literature showing discrepancies for some aluminum and boron compounds. Future work will extend tape coverage to more than 350 species, allow for variation of the form of the specific heat function and provide for updating of the data tape.

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NOLTR 62-84 15 May 1962

This report describes the construction of a magnetic tape library of thermodynamic data, for use with a high speed digital computer. The work was carried out as a part of the Naval Ordnance Laboratory's propellant development studies under Task PR-3, Propellant Formulation. The tape contains the data judged to be most reliable at the present time; it will be modified periodically to carry better data as they become available.

W. D. COLEMAN
Captain, USN
Commander

A. LIGHTBODY
By direction

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INTRODUCTION

The results presented in this report are a by-product of the Naval Ordnance Laboratory's effort in the field of rocket propellant research. Although taped thermodynamic data can be used for other problems, the tape was made specifically for use with a program* developed here to compute the theoretical performance parameters of solid rocket propellants. As is well known, the computation of specific impulse and other characteristic parameters of a propellant involves the use of large amounts of data for many chemical species; to be most useful for machine computation these data should be easily accessible, and amenable to simple modification if improved values are received. With the present state of the computer art, the use of a magnetic tape best fulfills the above requirements. Accordingly the objective was to collect, verify and collate thermodynamic data, and store them on a magnetic tape in a practical, accessible form.

For making the tape, the data fall into two categories: part, such as heats of formation, can be read onto the tape immediately after verification, while the remainder, such as specific heats, must be reduced to a form suitable for tape storage. Early workers tended to store data tables, giving values at discrete temperature values. Such data required interpolation for intermediate temperatures. A better practice is to reduce the data by a curve fitting process to a rational function of the temperature and store only the coefficients of the function. A Fortran language program, to be discussed later, was written and compiled to do this as well as other parts of the data work. After collection and preparation, the data were punched on cards and subsequently written onto an IBM magnetic tape. In this form they may be readily recalled for further work by the IBM 704 or 7090 computers. Sample Data Program output sheets are illustrated and discussed in the body of the report.

The various data sources searched agree with each other within one percent for the common compounds of carbon, hydrogen, nitrogen and oxygen and the common halides. In some cases, particularly with newer types of propellant ingredients e.g.,

*This program has been in operation since March 1960. It will be described in a forthcoming report.

light metals, the necessary data are not in final form as shown by the lack of agreement among competent workers in the field. Again, evidence of new species stable at high temperatures is being found and for these the data are still in the preliminary stage. More refined studies must be made on some ternary and higher compounds.

Although a data sheet has been printed out for verification for each species on the tape, it is not the intention here to add another member to the already large, and still growing list of published collections of thermodynamic data. Since most of these lists go back to a relatively few common sources such as reference (1), they represent duplication of effort in the case of the well known species and multiplication of inaccurracies in the case of newer ones. The latter require further effort to eliminate inaccurracies; discussion and selection of such data are better included in reports of work utilizing the particular quantities. For example, reported theoretical specific impulses should always be accompanied by input data on any questionable species considered in the calculations.

In the meantime, since there are differences between one laboratory and another in the calculational methods used, it would be helpful if all groups at least used common data. The JANAF Thermochemical Panel has undertaken the ambitious task of bringing this about; and one of the final objectives of the present work is to bring the data library tape into accord with the JANAF Thermochemical Tables. Further, coverage is being extended from 103 to about 350 chemical species and the program is being modified to allow more latitude in the treatment of specific heats and other data.

THEORY

As noted in Section I, the data to be recorded were divided into two parts: those to be taped immediately and those to be reduced first to a set of storable parameters. They were assembled mainly from the sources given by references 1 to 11. Data such as heats of formation, melting and boiling points were collected, verified, punched on IBM cards and read directly onto the magnetic tape.

For data from which thermodynamic functions were to be derived, the procedure was different; the items to be stored on

tape for each species were: coefficients of a function of the temperature, T, which defined the specific heat, C_p, at a pressure of one atmosphere, and two integration constants, H' and S', discussed below. From these data by the application of elementary thermodynamics, the enthalpy H, the entropy S and the Gibbs free energy G were derived.

Since C_p, an experimental quantity put into an appropriate analytical form, has to be integrated to obtain the enthalpy, it has to be represented by some function of T; and no one function provides a representation equally good for all chemical species. As pointed out by Maier and Kelley (12) it was at one time common practice to represent the enthalpy by an elementary power series in T, terms as high as T^3 usually being taken. Differentiation then resulted in a quadratic function for C_p which could, ".... have a maximum in the temperature range under consideration due to the signs and magnitudes of the coefficients, but such a maximum does not correspond to known physical facts". They proposed the addition of negative powers of the temperature, and showed by comparative results the improvement obtained over the simple quadratic function. Since then several different functions have been employed, with varying success, to represent $C_p(T)$ analytically. The form used here was noted in a Wright Air Development Center report (13), and has since been used in the preparation of the JANAF Thermochemical Tables (21). For all species they use the function

$$C_p = C_p(T) = a + b\theta + c\theta^2 + d\theta^3 + e\theta^{-2} \qquad (1)$$

where, for convenience

$$\theta = 10^{-3} T \qquad (2)$$

The problem was then to determine the set of parameters a, b, c, d and e for each chemical species. Obviously five equations were needed and these were obtained by using experimental values of C_p at five different temperatures. There resulted a set of five equations linear in a, b, c, d and e, and these were solved readily using a simple matrix inversion technique.

With a, b, c, d and e known for a species, C_p was defined; for the enthalpy and entropy, it remained only to determine the integration constants H' and S' respectively. The elementary

steps needed are summarized in Appendix A, and a detailed example was presented in reference (13). The variation of H' and S' was shown to be approximately 1% between 1000° and 6000°K. This was considered tolerable.

DATA COLLECTION

Although several score sources have been examined in the process of collecting thermodynamic data, only a few of the more important ones are referenced here (1 - 11). Of these, the most important were from the National Bureau of Standards (1, 4, 6, 7). The reference states of the elements were taken as given by Stull and Sinke (10).

Among the data in use, good agreement exists between one laboratory and another for the common compounds of carbon, hydrogen, nitrogen and oxygen, and also of fluorine and chlorine. However, when metallic combustion products are considered, agreement is often lacking between one laboratory and another. Present knowledge of these compounds has been summarized by Dobbins (9), pages 99 et seq; and Gilles (14) has reviewed the status of work on high temperature ternary species, another area where general agreement is lacking. It is necessary here only to present a few illustrative examples of variation in data used.

Fig. 1 shows three derived curves* of common log K vs 1/T for the reaction

$$Al_2O_3(l) + 2H_2(g) \longleftrightarrow Al_2O(g) + 2H_2O(l).$$

The upper and lower curves represented the extreme values among those based upon material in several classified and unclassified sources (2, 16, 17, 18, 19, 20). Since the scale on the ordinate represented powers of ten, the graph illustrated the large differences from one laboratory to another. The third curve shown was based upon values which are now considered acceptable, and are reported in the open literature (21).

*Before the publication of reference (15), flame temperatures and compositions were computed here using the older equilibrium constant method, thus the interest in log K. Although the method is no longer used, the results shown in Fig. 1 are typical of the kind of disagreement often found.

Another example is the standard heat of formation of boron nitride. This has been variously reported (in kcals per mol) as 131.4 (5), 155 (9) and 158.1 (1). Again the existence of a boron subchloride BCl_2 has been inferred (9) from the existence of the dimer; and the heat of formation of the subchloride has been reported as -24.6 (5) and -82.0 (9).

In cases such as these, the consistency of the given data with other known values for the species was checked. Until recently (See Recommendations) values given by the National Bureau of Standards were considered to be the most acceptable in cases which could not otherwise be decided. Henceforth, values from the JANAF tables will be used.

DATA CARD DECK

Six IBM cards are used to hold the data for each species prior to taping them. The first three cards (of the set of six) contain thermodynamic data and are described in Figs. 2, 3 and 4. Fig. 5 typifies the last three cards of the set. The summary of data for one species is indicated in Table 1. In this table the lower case letters, "cc" in the left hand column stand for, "card column" and define the card fields. The center column of the table lists the information in the corresponding card columns. The column on the right side of the table gives the storage designations for the data when they are being used. The letters SPD in this column originally meant Species Data, and are now used to identify all data storage designations.

The data for the first three cards of a set may be punched as soon as verified. The last three cards, typified by Fig. 5, refer to the gas (card 4), liquid (card 5) and solid (card 6) phases of a species. Each of these three contains seven numbers. The first five are respectively the coefficients a, b, c, d and e for the species and the last two are the corresponding integration constants H' and S', for the enthalpy and entropy respectively.

MACHINE PROGRAM

On page three and Appendix A equations are presented for the specific heat at constant pressure, the enthalpy, the entropy and Gibbs free energy as functions of temperature. A Fortran program was written to derive the coefficients of the C_p equation and to compute tables of these functions. A block diagram

of the program is shown in Fig. 6 and a copy of the Fortran listing is included as Appendix B.

Five options were built into the program, including one "dummy" for future use. The options have extended the program's usefulness. According to the job to be done, the proper option number was punched on a card and the program followed the indicated path. A description of the various options follows, in logical rather than numerical order.

Option (2). When new experimental C_p data were acquired, we wished to find the coefficients of the C_p function. The cards were punched as shown in Fig. 7. This option caused the program to compute a, b, c, d, e, H' and S', and print-out the results for inspection. Figure 8 is a sample of the print-out for this option showing the input C_p, H and S and the resulting set of constants.

Option (-1). If the data table derived from the above computed coefficients was desired, the cards for this option were punched as shown in Fig. 9 and used in conjunction with option (2). A sample of this output is shown in Fig. 10. The machine time for the example shown was approximately five seconds on the IBM 704.

Now if examination showed an error in the above table (Fig. 10) it was corrected at this point. If, however, the data were consistent with other known data, the new coefficients were punched on card No. 4, 5 or 6 for this species, depending upon the phase being considered and were now ready to be read onto the tape. In this way, the tape library was compiled. The tape is kept in the computer room, and the corresponding card deck is kept for use in future modifications of the tape.

Figures 11 and 12 illustrate the arrangement of the data on tape. It is exactly as the data card deck is read in. Fig. 11 shows the first cards (of each set of six) for several species. The identification numbers are in the left hand column, and the first forty rows were reserved for atomic species. A figure one occurs in the column corresponding to the identification number of the atomic species, i.e., row 12 has a one printed in column 12, row 14, a one printed in column 14, etc. This permitted a simple method of defining molecular types, which occupy the rows beyond number forty. For example, a one in row 7 identifies atomic hydrogen and a one in row 11 identifies atomic oxygen. So in order to specify a molecule of

H_2O (row 45), a 2 was placed in column 7 and a 1 in column 11. The assignment of a column to a particular element allowed efficient formulation of molecular species on tape. Upon recall of the data a Symbol Sub-routine identified the numbers in each row and converted them to atomic formulae. The remaining information (right hand columns of Fig. 12), includes the weights, given for atomic species only, and a set of numbers giving the references for each species.

Fig. 12 is a section of the print-out corresponding to the last five data cards for each of nine separate species. What appears are three rows for each species, corresponding to data cards 2, 3 and 4. This is because the species here listed do not have liquid (card 5) or solid (card 6) phases at the temperatures being considered. The full row in each group, shows in order a, b, c, d, e, H' and S' for the gas phase. If liquid or solid phases for any of these species were present, they would be placed in the two rows immediately below that for the gaseous phase. This option has been useful when a problem result indicated a possible error on the tape. It provides for fast checking.

Option (1). When it was desired to examine the tape contents, the input cards were punched as in Fig. 13. The print-out from this option consists of the taped information discussed above, listed with proper English column headings. It has been a convenient means of examining the tape contents.

Option (3). As in the other options, the cards used here (Fig. 14) were simple to prepare. The data tables for any species (Fig. 10), or chosen group of species, were obtained as the specific impulse program uses them. When desired, this option can print data tables for all the species on tape; such tables are in suitable form for publication.

In using the program, data cards are punched according to the appropriate figures for each option. The cards are then placed at the end of the program deck and run into the card hopper. Obviously, Options (-1) and (2) operate directly from card input, while (1) and (3) require that a data tape reel be placed on tape unit No. 7, the data input unit of the 704 computer. For the IBM 7090, the tape number is A7. If by the use

of Options (-1) and (2), acceptable species data have been generated, they are punched onto card 4, 5 or 6, and inserted into the library deck along with the first three cards for the species. In this way data on any species in the library deck can be replaced.

The library deck and the tape are the end results of the work. The program deck, used to handle the data, may be reproduced simply by punching the cards shown in the Fortran listing of Appendix B. After this program deck is compiled, it is necessary only to choose an option in order to use the system. Table 2 is a list of the 103 species for which data are on tape.

RESULTS

A continuing system has been set up for the acquisition, verification and recording on magnetic tape, of thermodynamic data. Methods have been developed for replacing data now on tape, and for adding data on new species. This work has been carried on simultaneously with work on the theoretical propellant calculation program so that a modicum of data was available as soon as the latter was ready to be tested. Much information has since been added to the library, and it has been used successfully for hundreds of propellant calculations. The Laboratory has not essayed the publication of a data book because the already long list of such books precludes further duplication. However, a print-out of the material on the tape has been made for our own use, and the latest tape revision occurred in May 1961.

It may be noted that the present method of storing thermodynamic data is a considerable improvement over older methods. Stored data tables are too unwieldy since it is at times desirable in a calculation to consider as many as 20 - 30 chemical species and the necessary table storage space is too large, even for modern memory devices. Besides this, the storage of data tables requires the use of interpolation subroutines since the occurrence of a temperature value lying between two of those given in the table is inevitable.

FUTURE WORK AND RECOMMENDATIONS

A better method of curve fitting might be used in the Fortran program. A least squares fit and Tchebicheff Polynomials are both being considered. Certain techniques which heretofore have been separate from the data program should be

assimilated into it as further options. For example, one separate program computes the coefficients a, b, c, d and e in equation (1) from coefficients as given by other C_p equations for the same species; while another program prints out all the data available at any given temperature, as a single block of information. Further, techniques are now available for providing relatively automatic updating of the tape. These techniques would allow an even simpler method of tape modification.

Since many species of great importance in rocket propellant calculations are still not completely defined, a continuing data search should be made for the most probable values among those available for these species.

In the past, the National Bureau of Standards data has been used as the most reliable. In the interest of furthering consistency among all groups in the field, the data used by this Laboratory should be based upon the data published by the JANAF Thermochemical Panel (21, 22). Revisions of these data are continually being supplied by the Panel; so the fact that the data in many cases is admittedly tentative should not be a deterrent.

Finally it would be of considerable interest to extend this work in the direction of more extreme thermodynamic conditions because of its potential use in explosives computations.

ACKNOWLEDGEMENT

Mr. William Evans of the Thermodynamics Division of the National Bureau of Standards has discussed parts of the work with the authors. Of those at the Naval Ordnance Laboratory, we are especially indebted to Dr. E. C. Noonan (deceased) and Dr. D. Price for critical appraisals of data on certain chemical species, and to Dr. Price and Mr. J. Enig for critical reading of the manuscript. In the Mathematical Computations Division the cooperation of Mr. H. Stevens and the IBM 704 Machine Operators has been appreciated; and without the very patient efforts of Mrs. Helena Hall, the transfer of data to punched cards would have been a much more painful process than it actually was. Finally, our thanks to Mrs. Mildred Ward for the typing of drafts and manuscripts.

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TABLE 1

Arrangement of Species Data

Card	Card Columns	Data	Tape
I	cc 1 ... 3	ID Number	SPD (I,1)
	cc 4 .. 43	Formulation	Not Stored
	cc 44 .. 53	Mol. Wt.	SPD(I,2)
	cc 54 (0.1)	Phase	SPD(I,3)
	cc 55 (1,..)	Ref.	Not Stored
II	cc 1 .. 10	ΔH_f^{298} (g)	SPD(I,4)
	cc 11 .. 20	ΔH_f^{298} (l)	SPD(I,5)
	cc 21 .. 30	ΔH_f^{298} (s)	SPD(I,6)
	cc 31 .. 40	bp	SPD(I,7)
	cc 41 .. 50	mp	SPD(I,8)
III	cc 1 .. 10	$H_{298}-H_o$ (g)	SPD(I,9)
	cc 11 .. 20	$H_{298}-H_o$ (l)	SPD(I,10)
	cc 21 .. 30	$H_{298}-H_o$ (s)	SPD(I,11)
	cc 31 .. 40	ΔH_v (vaporization)	SPD(I,12)
	cc 41 .. 50	ΔH_f(fusion)	SPD(I,13)
IV	cc 1 .. 10	a(g)	SPD(I,14)
	cc 11 .. 20	b	SPD(I,15)
	cc 21 .. 30	c	SPD(I,16)
	cc 31 .. 40	d	SPD(I,17)
	cc 41 .. 50	e	SPD(I,18)
	cc 51 .. 60	1H'	SPD(I,19)
	cc 61 .. 70	2S'	SPD(I,20)
V	cc 1 .. 10	a(l)	SPD(I,21)
	cc 11 .. 20	b	SPD(I,22)
	cc 21 .. 30	c	SPD(I,23)
	cc 31 .. 40	d	SPD(I,24)
	cc 41 .. 50	e	SPD(I,25)
	cc 51 .. 60	1H'	SPD(I,26)
	cc 61 .. 70	2S'	SPD(I,27)
VI	cc 1 .. 10	a(s)	SPD(I,28)
	cc 11 .. 20	b	SPD(I,29)
	cc 21 .. 30	c	SPD(I,30)
	cc 31 .. 40	d	SPD(I,31)
	cc 41 .. 50	e	SPD(I,32)
	cc 51 .. 60	H'	SPD(I,33)
	cc 61 .. 70	S'	SPD(I,34)

TABLE 2

List of Species on Tape

Al	HF	CF	BCl	LiCl
Al(l)	Cl_2	CF_2	BCl_2	LiF
B	ClF	CF_3	BCl_3	LiH
Be	HCl	CF_4	BF	LiO
C	ClO	C_2F_2	BF_3	Li_2O
C(s)	S_2	CF_3H	BH	LiOH
Cl	HS	CH_2F_2	BN	Al_2O
F	SO	CH_3F	BN(s)	AlF_3
H	N_2	COF_2	BO	AlF_2
Li	NFO	CH	B_2O_2	AlFO
Mg	NH	CH_2	B_2O_3	$AlCl_3$
N	NO	CH_4	AlF	$AlCl_3$(l)
O	P_2	CN	AlH	$AlCl_2$
P	P_4	C_2N_2	AlO	AlClO
S	PH	CNF	Al_2O_3(l)	$AlClF_2$
Si	PH_3	CO	Al_2O_3(s)	AlClF
O_2	PN	CO_2	BeF	AlCl
O_3	PO	COH_2	BeH	AlC
H_2	C_2	CP	BeO	AlF
OH	C_3	CS	MgF	AlS
H_2O	CCl	SiO	MgH	
F_2	$COCl_2$	B_2	Li_2	

NOTE: All species are gaseous unless noted, in which cases an s or l in parenthesis indicates the solid or liquid phase respectively.

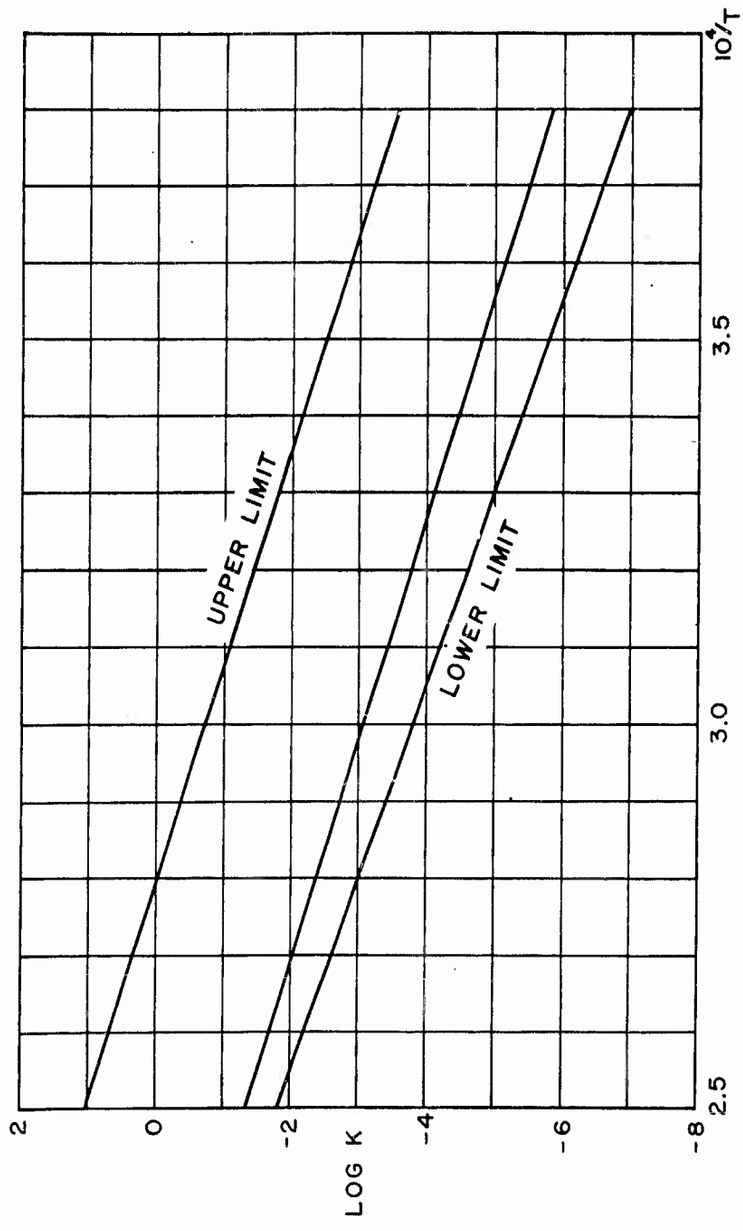
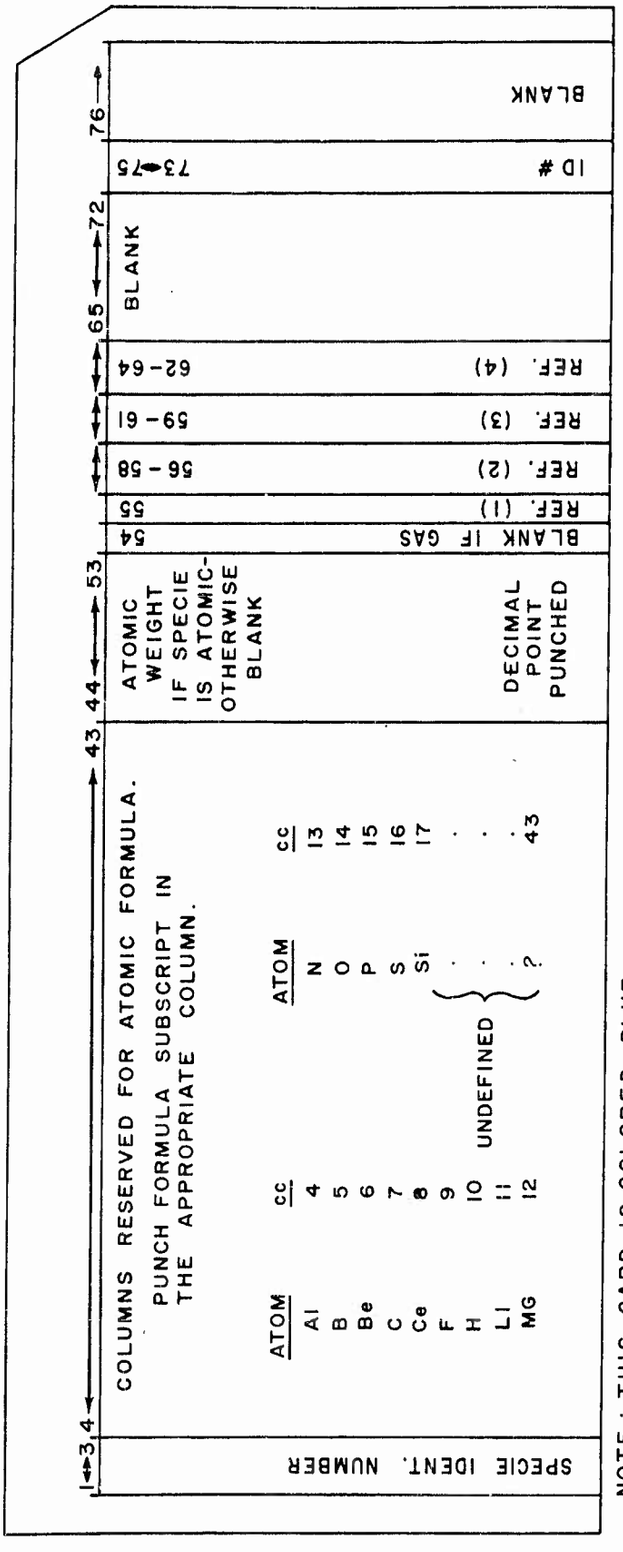
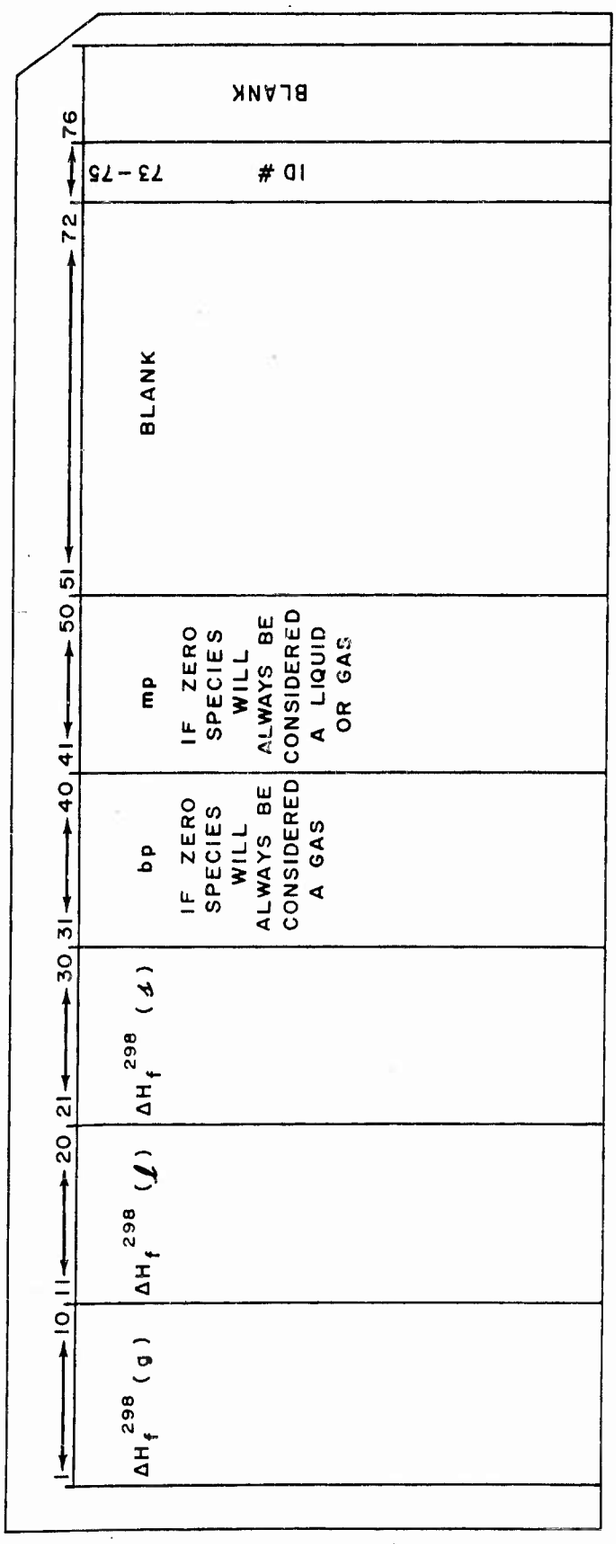


FIG. 1 LOG K VS $^1/_T$ FOR THE REACTION OF $Al_2O_3(\ell)$ AND $H_2(g)$



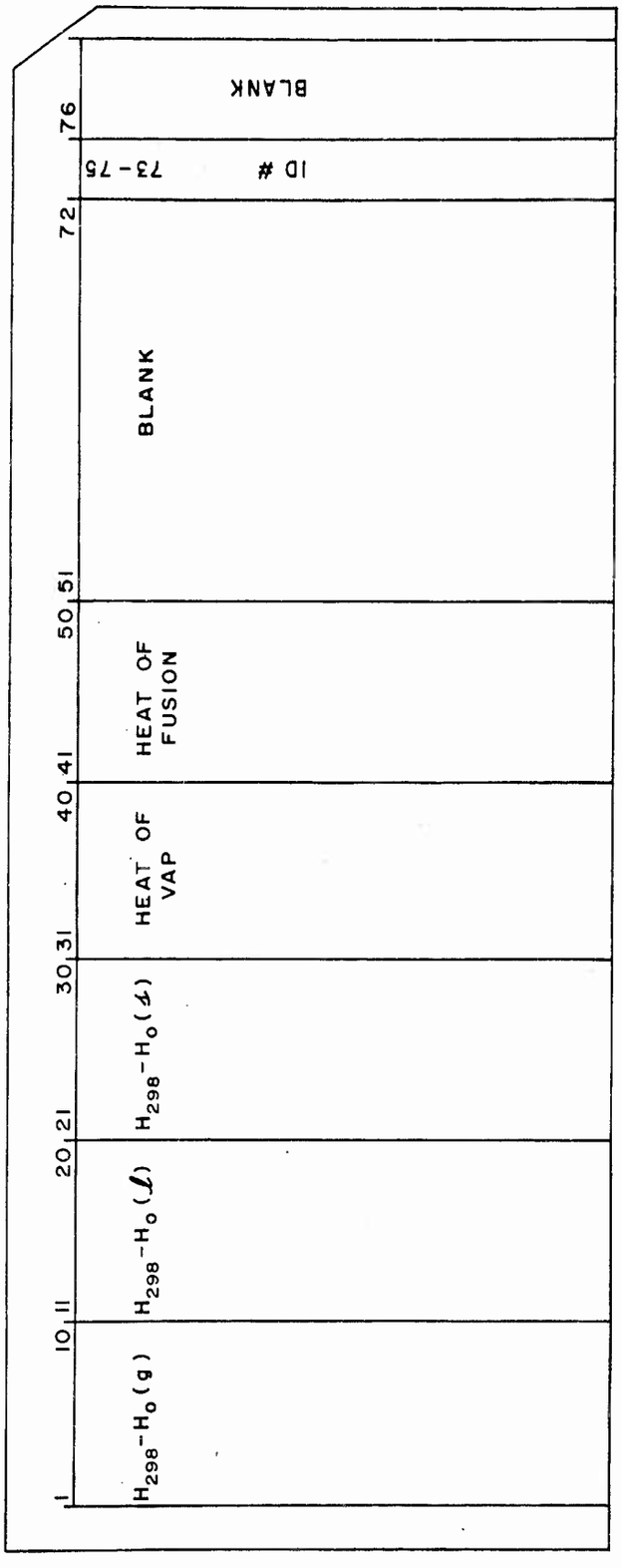
NOTE: THIS CARD IS COLORED BLUE.

FIG. 2 INFORMATION ON DATA CARD NO. 1



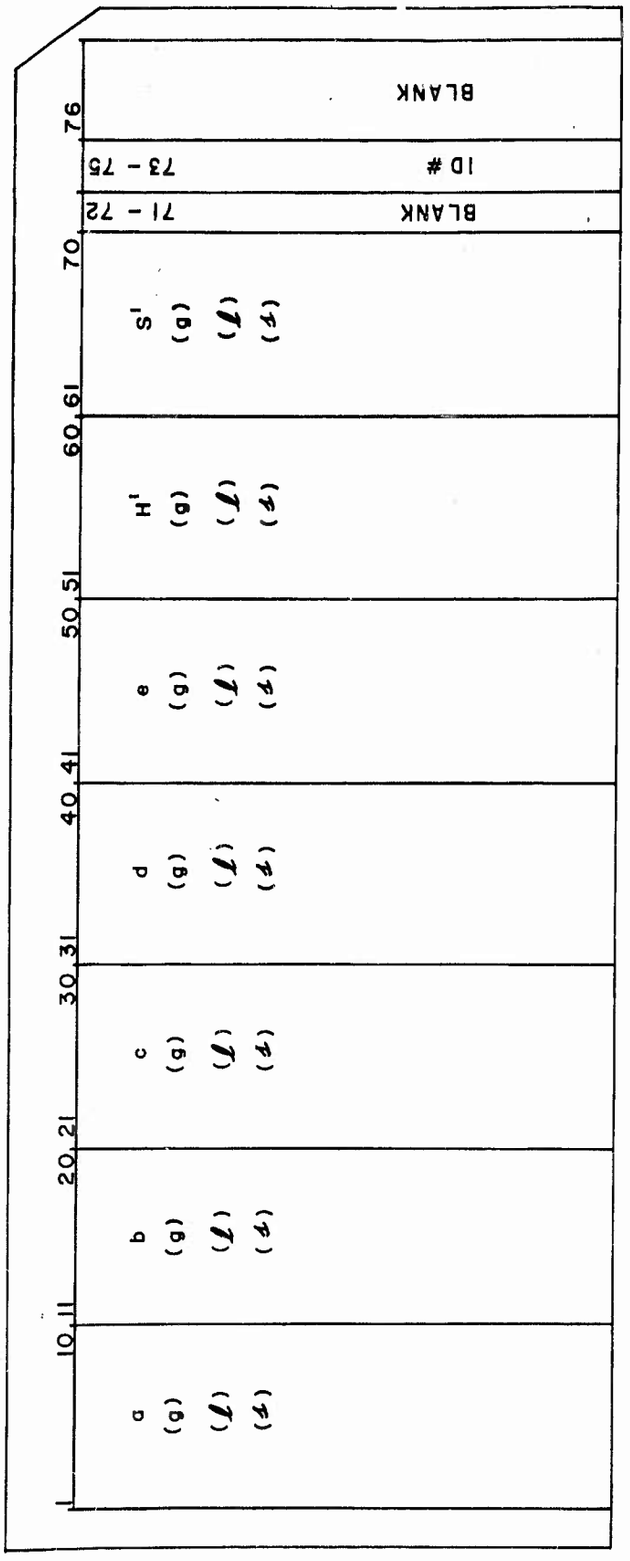
NOTE : THIS CARD IS COLORED YELLOW.
DECIMAL POINT PUNCHED FOR EACH DATUM.

FIG. 3 INFORMATION ON DATA CARD NO. 2



NOTE : THIS CARD IS COLORED YELLOW.
DECIMAL POINT PUNCHED FOR EACH DATUM.

FIG. 4 INFORMATION ON DATA CARD NO. 3



NOTE: THESE CARDS ARE COLORED YELLOW.
DECIMAL POINT PUNCHED FOR EACH DATUM.
CARD NUMBER 4 IS FOR GAS PHASE.
CARD NUMBER 5 IS FOR LIQUID PHASE.
CARD NUMBER 6 IS FOR SOLID PHASE.

FIG. 5 INFORMATION ON DATA CARDS NOS. 4, 5 AND 6

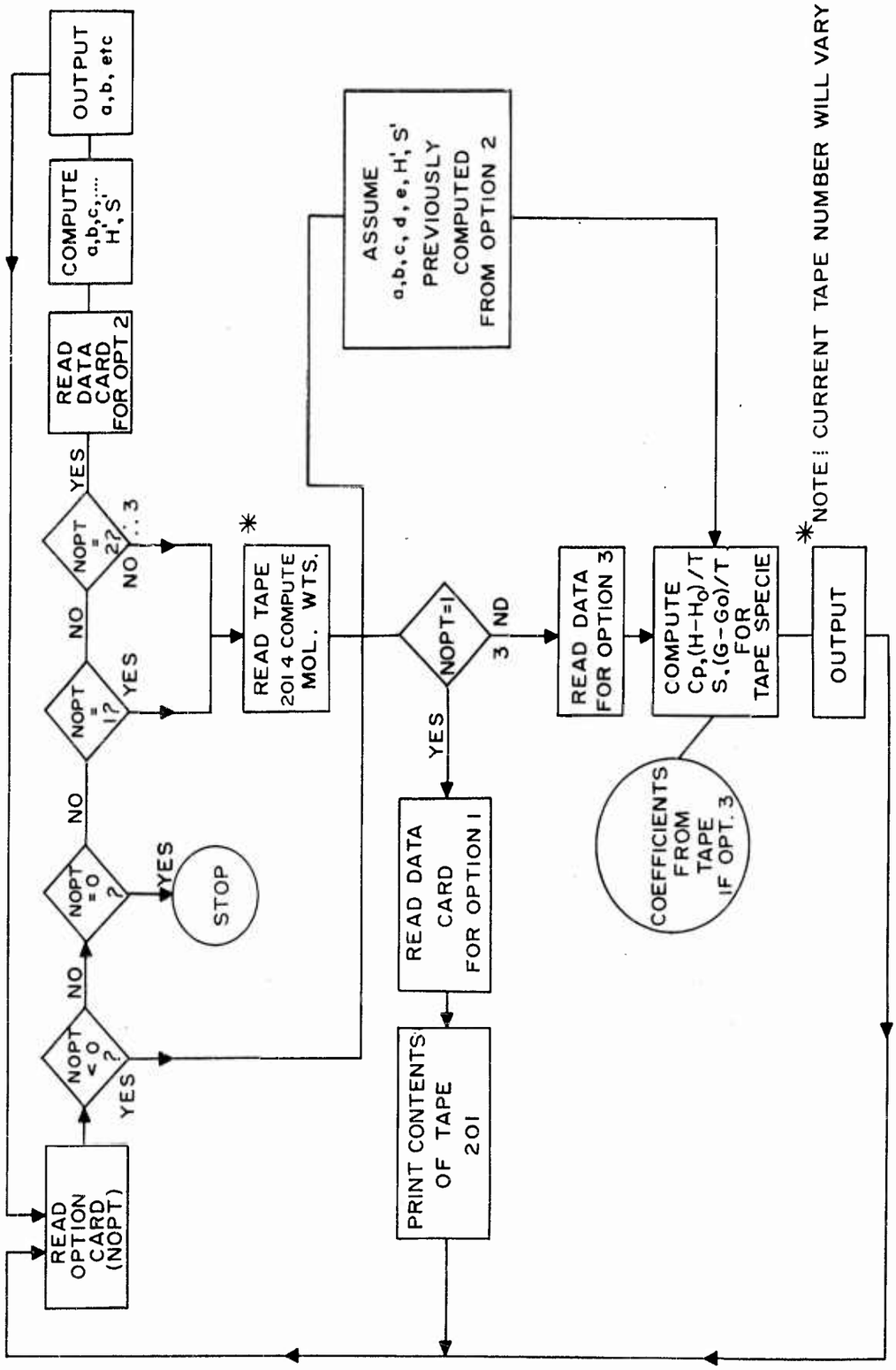


FIG. 6 BLOCK DIAGRAM OF MACHINE PROGRAM

THREE CARDS ARE USED FOR THIS OPTION

Card No. 1:

cc 2, punch: 2

Card No. 2:

punch: Δ coefficient Δ determination Δ for H_2O Δ formula (atomic formula of species)

Card No. 3:

cc 1-10	punch:	$C_p(1000)$
cc 11-20	punch:	$C_p(1600)$
cc 21-30	punch:	$C_p(3000)$
cc 31-40	punch:	$C_p(4500)$
cc 41-50	punch:	$C_p(5700)$
cc 51-60	punch:	H'(3000)
cc 61-70	punch:	S'(3000)

Note: On Card No. 2 Δ represents a blank. cc means card column.
Fixed point: decimal point must be punched.

Figure 7 - Input Cards for Option (2)

COEFFICIENT DETERMINATION FOR $H2O_{(g)}$

MATCH TEMPERATURES	1000	1600	3000	4500	5700
CP	9.851	11.462	13.304	14.030	14.351

(H(3000)-H(0))/3000 = 10.856

S(3000) = 68.421

a	b	c	d	e	H^{I}	S^{I}
7.74325E 00	3.40507E 00	6.36411E-01	4.26448E-02	-7.03557E-01	-1.35496E 00	5.21399E 01

NOTE: TRIAL COEFFICIENT DETERMINATION BASED UPON DATA FROM JANAF THERMOCHEMICAL TABLES; IN THIS CASE, ENTHALPY AND ENTROPY VALUES WERE TAKEN ONLY AT 3000° K

FIG.8 OUTPUT FROM OPTION 2

TWO CARDS ARE USED FOR THIS OPTION

Card No. 1

cc 1, 2 punch: -1

Card No. 2

cc 1-10 punch: T_i

cc 11-20 punch: T_f

cc 21-30 punch: ΔT

NOTE: T_i and T_f are the lower and upper limits of the temperature interval over which data are desired. ΔT is the size of the step from T_i to $T_{(i + 1)}$

NOTE: Fixed point: decimal point must be punched.

Figure 9 - Input Cards for Option (-1)

THERMODYNAMIC DATA FOR H_2O GAS

T (°Kelvin)	CP (CALS/ MOL °K)	$(H-H_o)/T$ (CALS/ MOL °K)	S (CALS/ MOL °K)	$(G-G_o)/T$ (CALS/ MOL°K)
1000.	9.85026E 00	8.57754E 00	5.55906E 01	-4.70131E 01
1100.	1.01561E 01	8.70725E 00	5.65149E 01	-4.78077E 01
1200.	1.04474E 01	8.84023E 00	5.73839E 01	-4.85437E 01
1300.	1.07229E 01	8.97455E 00	5.82045E 01	-4.92299E 01
1400.	1.09823E 01	9.10880E 00	5.89822E 01	-4.98734E 01
1500.	1.12256E 01	9.24190E 00	5.97214E 01	-5.04795E 01
1600.	1.14530E 01	9.37307E 00	6.04258E 01	-5.10527E 01
1700.	1.16649E 01	9.50172E 00	6.10983E 01	-5.15966E 01
1800.	1.18619E 01	9.62744E 00	6.17414E 01	-5.21140E 01
1900.	1.20444E 01	9.74991E 00	6.23574E 01	-5.26075E 01
2000.	1.22132E 01	9.86891E 00	6.29481E 01	-5.30792E 01
2100.	1.23689E 01	9.98430E 00	6.35151E 01	-5.35308E 01
2200.	1.25122E 01	1.00960E 01	6.40598E 01	-5.39639E 01
2300.	1.26439E 01	1.02039E 01	6.45837E 01	-5.43797E 01
2400.	1.27646E 01	1.03082E 01	6.50877E 01	-5.47796E 01
2500.	1.28752E 01	1.04087E 01	6.55731E 01	-5.51644E 01
2600.	1.29765E 01	1.05055E 01	6.60406E 01	-5.55351E 01
2700.	1.30691E 01	1.05988E 01	6.64913E 01	-5.58926E 01
2800.	1.31539E 01	1.06885E 01	6.69259E 01	-5.62374E 01
2900.	1.32316E 01	1.07749E 01	6.73452E 01	-5.65703E 01
3000.	1.33032E 01	1.08580E 01	6.77499E 01	-5.68919E 01
3100.	1.33692E 01	1.09380E 01	6.81406E 01	-5.72026E 01
3200.	1.34306E 01	1.10149E 01	6.85180E 01	-5.75031E 01
3300.	1.34881E 01	1.10890E 01	6.88826E 01	-5.77937E 01
3400.	1.35425E 01	1.11604E 01	6.92351E 01	-5.80748E 01
3500.	1.35947E 01	1.12292E 01	6.95760E 01	-5.83468E 01
3600.	1.36453E 01	1.12956E 01	6.99058E 01	-5.86102E 01
3700.	1.36954E 01	1.13598E 01	7.02249E 01	-5.88651E 01
3800.	1.37455E 01	1.14219E 01	7.05339E 01	-5.91120E 01
3900.	1.37966E 01	1.14821E 01	7.08332E 01	-5.93511E 01
4000.	1.38494E 01	1.15406E 01	7.11233E 01	-5.95826E 01
4100.	1.39047E 01	1.15976E 01	7.14045E 01	-5.98069E 01
4200.	1.39634E 01	1.16532E 01	7.16774E 01	-6.00242E 01
4300.	1.40263E 01	1.17077E 01	7.19424E 01	-6.02347E 01
4400.	1.40941E 01	1.17611E 01	7.21997E 01	-6.04386E 01
4500.	1.41676E 01	1.18138E 01	7.24499E 01	-6.06361E 01

NOTE: Given the necessary coefficients, compute and print data table for species named, from 1000°K to 6000°K.

FIG. 10 PARTIAL OUTPUT FROM OPTION (-1)

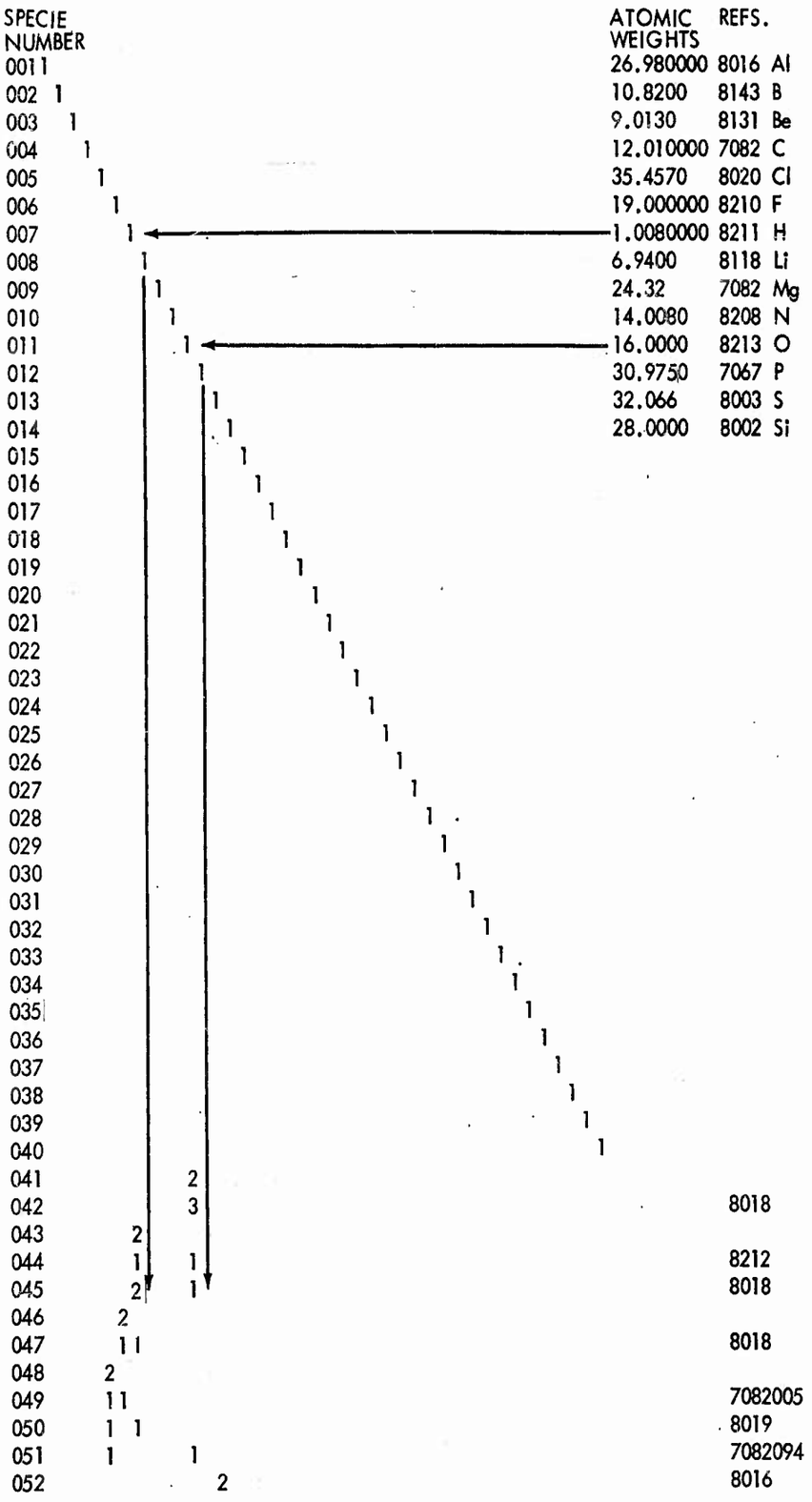


FIG. II INPUT TAPE LISTING (A)

CARD NO.							
2	121600.						
3	2250.						
4	8.91979	0.04404	-0.00241	0.00017	-0.19660	-0.9700	63.8156
5							
6							
2	-53300.			264.7			
3	3283.						
4	18.5699	1.01499	-.28713	.02781	-.73558	-4.3637	88.2420
5							
6							
2	74500.						
2	2170.						
4	8.59423	0.36810	-0.08798	0.00895	-0.34429	-1.3240	59.8720
5							
6							
2	-30000.						
3	2467.						
4	13.52244	0.24640	-0.05383	0.00372	-0.87872	-3.9585	70.2310
5							
6							
2	-120500.						
3	2794.						
4	18.97333	0.70465	-0.20308	0.02012	-1.2850l	-6.4394	79.8664
5							
6							
2	-218000.						
3	3045.						
4	24.72236	0.87981	-0.25485	0.02539	-1.74270	-9.2157	84.9078
5							
5							
2	-51300.						
3	3293.						
4	19.13848	2.55046	-0.37588	0.03702	-1.04807	-5.2626	78.9155
5							
6							
2	-162600.						
3	2765.						
4	21.26435	3.33827	-0.91481	0.08746	-2.04527	-0.1818	78.9034
5							
6							
2	-1.05500.						
3	2556.						
4	17.92884	5.77349	-1.58420	0.15200	-2.30013	-8.8788	70.8631
5							
6							

NOTE: Rows numbered 2 contain $\Delta H_f^\circ(g)$ for each species.
Rows numbered 3 contain $(H_{298}-H_0)$ (g) for each species.
Rows numbered 4 contain a, b, c, d, e, H' and S' for gas phase.
Rows numbered 5 and 6 are blank, since only gas phases are important for the above species.

FIG. 12 INPUT TAPE LISTING (B)

TWO CARDS ARE USED FOR THIS OPTION

Card No. 1

cc 2 punch: 1

Card No. 2

Start in cc 1, and punch as follows:

xx	Δ	xx	Δ	xx
month		Day		Year

NOTE: Δ on Card No. 2 represents a blank

Figure 13 - Input for Option (1)

TWO CARDS ARE USED FOR THIS OPTION

Card No. 1

cc 2 punch: 3

Card No. 2

cc 1, 2, 3	punch:	identification number
cc 4	punch:	g, l, or s (phase)
cc 5, 14	punch:	T_i
cc 15, 24	punch:	T_f
cc 25, 34	punch:	ΔT

NOTE: Fixed point: decimal point must be punched.

Figure 14 - Input Cards for Option (3)

APPENDIX A

Equations Used by the Program

Equation (1), Section II, defines $C_p(T)$ at a pressure of one atmosphere; and from Equation (2)

$$dT = 10^3 d\theta \ .$$

The enthalpy is then obtained by integrating

$$dH = C_p dT = 10^3 C_p d\theta \quad ; \tag{A1}$$

thus

$$H = 10^3 a\theta + \frac{10^3 b\theta}{2}^2 + \frac{10^3 c\theta}{3}^3 + \frac{10^3 d\theta}{4}^4 - \frac{10^3 e}{\theta} + H', \tag{A2}$$

where H' is the constant of integration.

Dividing Equation (A2) by $T = 10^3$ gives the enthalpy per degree. It is convenient to define

$$\frac{H - H_o}{T} = a + \frac{b\theta}{2} + \frac{c\theta}{3}^2 + \frac{d\theta}{4}^3 - e\theta^{-2} + \frac{H' - H_o}{10^3} \tag{A3}$$

Where the subscript o refers to the thermodynamic state at one atmosphere pressure and absolute zero of temperature. The integration constant used is an average value determined from

$$H' = \frac{1}{n} \sum_{i=1}^{n} H_i(T_i); \tag{A4}$$

where $H_i(T_i)$ is the i^{th} integration constant, obtained by substituting the i^{th} temperature and enthalpy into Equation (A2) and n is the number of such substitutions.

For a reversible process at constant pressure the entropy change is

$$dS = \left(\frac{dH}{T}\right)_P \ , \tag{A5}$$

where S is the entropy. Using Equation (A1) and again taking the indefinite integral gives

$$S = a\ln\theta + b\theta + \frac{c\theta}{2}^2 + \frac{d\theta}{3}^3 - \frac{e\theta}{2}^{-2} + S' , \qquad (A6)$$

where the integration constant S' is determined in the same way as H'.

Using the Gibbs free energy

$$G = H - TS$$

it is convenient to tabulate

$$-\frac{(G - G_o)}{T} = S - \frac{(H - H_o)}{T} \qquad (A7)$$

where S_o has been arbitrarily chosen as zero.

Using Equations (1),(A3) and (A5) for C_p, $(H - H_o)/T$ and S respectively made the machine computations unnecessarily cumbersome. Simple algebraic manipulaticns (nesting) resulted in the more economical forms,

$$C_p = e/\theta^2 + a + \theta\left[b + \theta(c + d\theta)\right] \qquad (A8)$$

$$\frac{H - H_o}{T} = \frac{1}{\theta}\left[\frac{H'}{10^3} - \frac{e}{\theta}\right] + a + \theta\left[\frac{b}{2} + \theta\left(c/3 + d\theta/4\right)\right] \qquad (A9)$$

$$S = S' - \frac{e0}{2}^{-2} + a\ln\theta + \theta\left[b + \theta\left(c/2 + \frac{\theta d}{3}\right)\right] \qquad (A10)$$

APPENDIX B

Fortran Listing

For those who wish to use it, the Fortran source program is given here. It is necessary only to punch the instructions on Hollerith cards, ignoring the blanks inserted before each Option.

Five comments occur in the listing. They are marked by a "C" in column one, and are in correct format. They will not interfere with the operation of the program, and are inserted to emphasize the Options. On page 5 the letter B occurring in column one identifies Boolean instructions. All others are in FortranII language.

No control instructions are shown since they depend upon the system being used at a particular installation.

THERMODYNAMIC DATA PROGRAM

```
C       CHOOSE AN OPTION
        DIMENSION SPD(300,34),FORM(40),NREF(300,4),CP(5),A(5,5),C(5)
SXGAS ALF   G
SXLIQ ALF   L
 31     READ1,NOPT
 1      FORMAT(I2)
        IF(NOPT)19,30,2
 2      GO TO (3,13,3,1000),NOPT
 1000   GO TO 3
 3      IF(SPD(1,1))3001,3000,3001
 3000   READ INPUT TAPE 7,4,(SPD(I,1),(FORM(J),J=1,40),SPD(I,2),
       1SPD(I,3),(NREF(I,K),K=1,4),I=1,40)
 4      FORMAT(F3.0,40F1.0,F10.0,2I1,3I4)
        DO 1001 I=41,300
        READ INPUT TAPE 7,4,SPD(I,1),(FORM(J),J=1,40),SPD(I,2),
       1SPD(I,3),(NREF(I,K),K=1,4 )
        DO 1001 J=1,40
 1001   SPD(I,2)=SPD(I,2)+FORM(J)*SPD(J,2)
        READ INPUT TAPE 7,1002,((SPD(I,J),J=4,34),I=1,300)
 1002   FORMAT(5F10.0/5F10.0/7F10.0/7F10.0/7F10.0)
        REWIND 7
 3001   GO TO (6,6,22),NOPT


C       BEGIN OPTION 1
 6      READ 7,MO,NDAY,NYEAR
 7      FORMAT(I2,2I3)
        PRINT 8,MO,NDAY,NYEAR
 8      FORMAT(111H1LISTING OF SPECIE-DATA INPUT (TAPE7) TO THEORETICAL PE
       1RFORMANCE PROGRAM                                          I2,1H/I2,1
       1H/I2)
        PRINT 9
 9      FORMAT(103H1                                  B.P.     M.P.      HV          HM
       1        HF(298) (KCAL/KMOL)                      REFERENCES/84H
       1          (K)      (K)         (KCAL/KMOL)        (G)         (L)
       1 (S)/22H SPECIE ID.NO. MOL.WT.)
        NPAGE=0
        DO 11 I=1,300
        ID=SPD(I,1)
        PRINT 10,ID,SPD(I,2),SPD(I,7),SPD(I,8),
       1SPD(I,12),SPD(I,13),SPD(I,4),SPD(I,5),SPD(I,6),(NREF(I,J),J=1,4)
 10     FORMAT(9H          I3,F9.3,2F8.1,5F10.0,3H   I1,2H, I3,2H, I3,2H, I
       13)
        CALL SYMBOL(I,2,NCH)
        NPAGE=NPAGE+1
        IF(NPAGE-50)11,1005,1005
 1005   NPAGE=0
        PRINT 9
```

```
11    CONTINUE
      PRINT 1007
1007 FORMAT(83H1                                  H(298)-H(0)
     1                COEFFICIENTS/102H SPECIE ID.NO. PHASE     (KCAL/KMOL
     1)            A          B          C          D          E        K1
     1K2)
      N=0
      NPAGE=0
      DO 1008 I=1,300
      TEST G=0.
      TEST L=0.
      TEST S=0.
      ID=SPD(I,1)
      DO 1009 K=1,7
      TESTG=SPD(I,K+13)+TESTG
      TESTL=SPD(I,K+20)+TESTL
1009 TESTS=SPD(I,K+27)+TESTS
      IF(NPAGE-47)1021,1020,1020
1020 NPAGE=0
      PRINT 1007
1021 IF(TESTG)1012,1010,1012
1010 IF(TESTL)1014,1011,1014
1011 IF(TESTS)1016,1018,1016
1012 PRINT 1013,ID,SPD(I,9),(SPD(I,J+13),J=1,7)
1013 FORMAT(9H          I3,15H    (G)         F5.0,12H             ,
     15F9.5,F8.4,F9.4)
      NPAGE=NPAGE+1
      CALL SYMBOL (I,2,NCH)
      GO TO 1010
1014 PRINT 1015,ID,SPD(I,10),(SPD(I,J+20),J=1,7)
1015 FORMAT(9H          I3,15H    (L)         F5.0,12H             ,
     15F9.5,F8.4,F9.4)
      NPAGE=NPAGE+1
      CALL SYMBOL (1,2,NCH)
      GO TO 1011
1016 PRINT 1017,ID,SPD(I,11),(SPD(I,J+27),J=1,7)
1017 FORMAT(9H          I3,15H    (S)         F5.0,12H             ,
     15F9.5,F8.4,F9.4)
      NPAGE=NPAGE+1
      CALL SYMBOL(I,2,NCH)
      GO TO 1018
1018 IF(TESTG+TESTL+TESTS) 1019,1008,1019
1019 N=N+1
1008 CONTINUE
      PRINT 2000,N
2000 FORMAT(22H0DATA IS AVAILABLE FOR I4,9H SPECIES.)
      GO TO 31


C      BEGIN OPTION 2
 13   READ 14
 14   FORMAT(37H COEFFICIENT DETERMINATION FOR          )
      READ 17,(CP(I),I=1,5),H,S
 17   FORMAT(7F10.0)
```

```
      A(1,1)=-3.2040805
      A(1,2)=10.955440
      A(1,3)=-12.815569
      A(1,4)=8.7032594
      A(1,5)=-2.6390499
      A(2,1)=1.9376145
      A(2,2)=-7.2087899
      A(2,3)=10.775001
      A(2,4)=-8.0360433
      A(2,5)=2.5322178
      A(3,1)=-0.41001527
      A(3,2)=1.6033583
      A(3,3)=-2.7948590
      A(3,4)=2.4161851
      A(3,5)=-0.81466908
      A(4,1)=0.029156571
      A(4,2)=-.11770102
      A(4,3)=0.22712088
      A(4,4)=-0.22307338
      A(4,5)=0.08449696
      A(5,1)=2.6473247
      A(5,2)=-5.2323073
      A(5,3)=4.6083062
      A(5,4)=-2.8603279
      A(5,5)=0.8370043
      DO 15 I=1,5
      C(I)=0.
      DO 15 J=1,5
 15   C(I)=A(I,J)*CP(J)+C(I)
      XK1=3.*H-3.*C(1)-4.5*C(2)-9.*C(3)-20.25*C(4)+C(5)/3.
      XK2=S-1.09861*C(1)-3.*C(2)-4.5*C(3)-9.*C(4)+C(5)/18.
      PRINT 16
 16   FORMAT(1H1)
      PRINT 14
 117  PRINT 18,(CP(I),I=1,5),H,S,(C(I),I=1,5),XK1,XK2
 18   FORMAT(71H0      MATCH TEMPERATURES       1000     1600     3000
     1  4500     5700/27H                        CP  5F9.3/28H0      (H(3
     1000)-H(0))/3000 =F8.3/25H                  S(3000) =F8.3/105H0
     1             A              B              C             D
     1   E            K1            K2/12H           1P7E14.5)
      GO TO 31


C      BEGIN OPTION -1
 19   READ 20,TZ,TF,DT
 20   FORMAT(3F10.0)
      PRINT 21
 21   FORMAT(45H1THERMODYNAMIC FUNCTIONS FOR THE ABOVE SPECIE)
      GO TO 26
```

```
C       BEGIN OPTION 3
 22     READ 23,NSP,PHASE,TZ,TF,DT
 23     FORMAT(I3,1A1,3F10.0)
B       TESTG=(PHASE+XGAS)*(-(PHASE*XGAS))
B       TESTL=(PHASE+XLIQ)*(-(PHASE*XLIQ))
       IF(TESTG) 1022,1023,1022
 1022  IF(TESTL) 1024,1025,1024
 1023  J=13
       GO TO 1026
 1025  J=20
       GO TO 1026
 1024  J=27
 1026  DO 24 I=1,5
       K=I+J
 24    C(I)=SPD(NSP,K)
       XK1=SPD(NSP,J+6)
       XK2=SPD(NSP,J+7)
       IF(TESTG) 1027,1030,1027
 1027  IF(TESTL) 1028,1029,1028
 1030  PRINT 1031
       GO TO 1034
 1029  PRINT 1032
       GO TO 1034
 1028  PRINT 1033
       GO TO 1034
 1031  FORMAT(39H1THERMODYNAMIC FUNCTIONS FOR         (G))
 1032  FORMAT(39H1THERMODYNAMIC FUNCTIONS FOR         (L))
 1033  FORMAT(39H1THERMODYNAMIC FUNCTIONS FOR         (S))
 1034  CALL SYMBOL(NSP,30,NCH)
       GO TO 26
 26    PRINT 27
 27    FORMAT(97H0         T                    CP                (H-H(0))/T
      1                S                (G-G(0))/T)/97H          (K)
      1  (KCAL/KMOL-K)        (KCAL/KMOL-K)          (KCAL/KMOL-K)         (KC
      1AL/KMOL-K)/1H )
       NSTOP=1.+(TF-TZ)/DT
       DO 28 I=1,NSTOP
       XI=I
       T=TZ+(XI-1.)*DT
       THETA=T/1000.
       CPZ=C(1)+THETA*(C(2)+THETA*(C(3)+THETA*C(4)))+C(5)/THETA**2
       HOT=XK1/THETA+C(1)+.5*C(2)*THETA+.33333333*C(3)*THETA**2+.25
      1*C(4)*THETA**3-C(5)/THETA**2
       SZ=XK2+C(1)*LOGEF(THETA)+C(2)*THETA+.5*C(3)*THETA**2+.33333333
      1*C(4)*THETA**3-C(5)/2.*THETA**2
       GZ=HOT-SZ
 28    PRINT 29,T,CPZ,HOT,SZ,GZ
 29    FORMAT(6H       F6.0,3H    1P4E20.5)
       GO TO 31
 30    CALL ENDJOB
```

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Naval Ordnance Laboratory, White Oak, Md. (NOL technical report 62-84)
A MAGNETIC TAPE LIBRARY OF THERMODYNAMIC DATA(U), by Bernard A. Burke and others. 15 May 1962. 25p. tables, charts, diags. Task PR-3.

UNCLASSIFIED

This report describes the production and use of a magnetic tape library of thermodynamic data. The tape is produced from a deck of punched cards. The data on each species include an identification number, coded references, formula, and atomic weight, the enthalpy change from 0°K to 298.15°K, the standard heat of formation at 298.15°K, melting point and heat of fusion, boiling point and heat of vaporization, coefficients giving the specific heat as a rational function of the temperature, and integration constants permitting calculation of enthalpy and entropy.

1. Thermodynamic
2. Chemicals - Thermodynamic properties
3. Mathematical computer data - Processing

I. Title
II. Burke, Bernard A.
III. Project

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Naval Ordnance Laboratory, White Oak, Md. (NOL technical report 62-84)
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